LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021924\
Data File : VN081084.D
Acq On : 19 Feb 2024 18:29
Operator : JC\MD
Sample : P1528-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
IDW-20240215

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Title : SW846 8260

Signal : TIC: VN081084.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.395	60	75	93	rBV	1846391	4977975	79.76%	15.943%
2	2.818	139	147	148	rBV	42033	91783	1.47%	0.294%
3	6.042	683	695	697	rBV	2108630	6240854	100.00%	19.988%
4	6.065	697	699	718	rVB	2847000	3340634	53.53%	10.699%
5	7.953	1016	1020	1025	rBV2	54179	86536	1.39%	0.277%
6	8.024	1025	1032	1033	rBV3	83212	164506	2.64%	0.527%
7	8.447	1095	1104	1106	rBV2	306211	693447	11.11%	2.221%
8	8.483	1106	1110	1116	rVB	446075	901222	14.44%	2.886%
9	8.818	1161	1167	1176	rVB	308672	658970	10.56%	2.111%
10	9.053	1197	1207	1222	rVB	1768076	4267771	68.38%	13.669%
11	9.288	1239	1247	1254	rBV	759320	1512132	24.23%	4.843%
12	10.659	1472	1480	1494	rBV	885439	1711393	27.42%	5.481%
13	11.912	1685	1693	1706	rBV	814535	1522631	24.40%	4.877%
14	12.118	1722	1728	1734	rVB2	44806	89973	1.44%	0.288%
15	12.871	1848	1856	1865	rVB	608997	1099076	17.61%	3.520%
16	13.059	1883	1888	1893	rVB3	40274	67651	1.08%	0.217%
17	13.147	1897	1903	1907	rVV2	42425	74480	1.19%	0.239%
18	13.353	1932	1938	1947	rVB2	63130	113000	1.81%	0.362%
19	13.659	1975	1990	2008	rVV3	118525	775914	12.43%	2.485%
20	13.806	2008	2015	2025	rVB2	797240	1595186	25.56%	5.109%
21	14.006	2043	2049	2060	rVB	212471	408629	6.55%	1.309%
22	14.188	2073	2080	2086	rBV6	35047	75382	1.21%	0.241%
23	14.247	2086	2090	2100	rVV6	31963	81322	1.30%	0.260%
24	15.059	2220	2228	2234	rVB5	36461	84771	1.36%	0.271%
25	15.212	2247	2254	2266	rBV	230244	434968	6.97%	1.393%
26	15.753	2340	2346	2354	rBV2	29737	67409	1.08%	0.216%
27	16.723	2501	2511	2518	rBV5	27469	85653	1.37%	0.274%

Sum of corrected areas: 31223268

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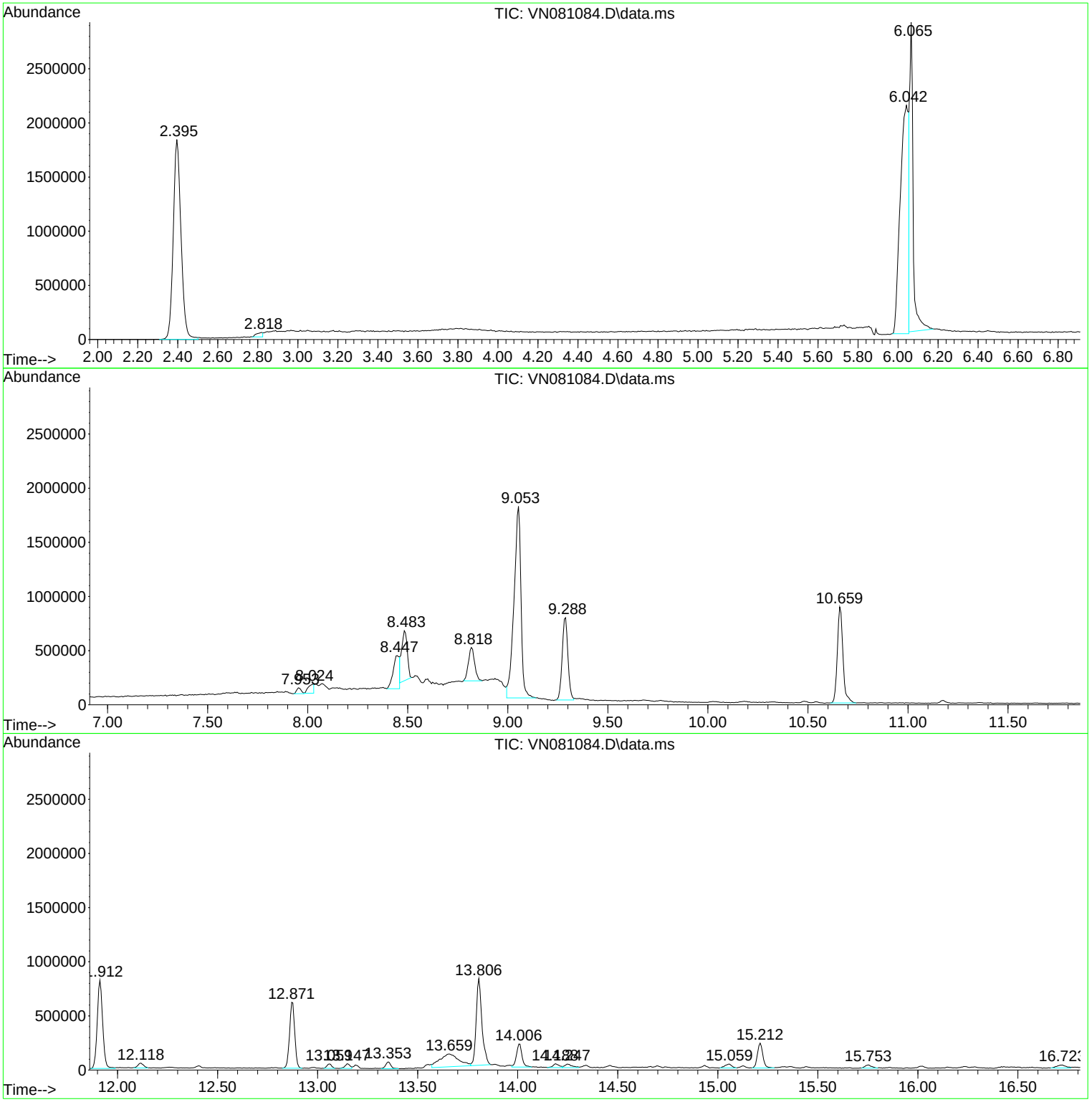
Instrument :
MSVOA_N
ClientSampleId :
IDW-20240215

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Operator : JC\MD
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

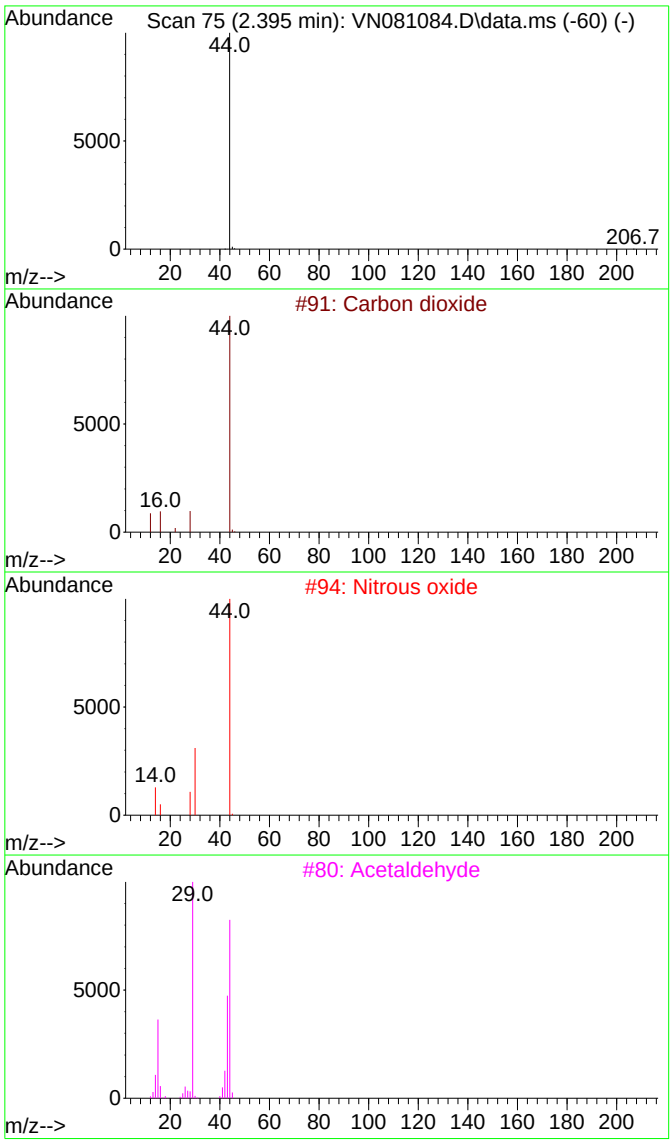
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

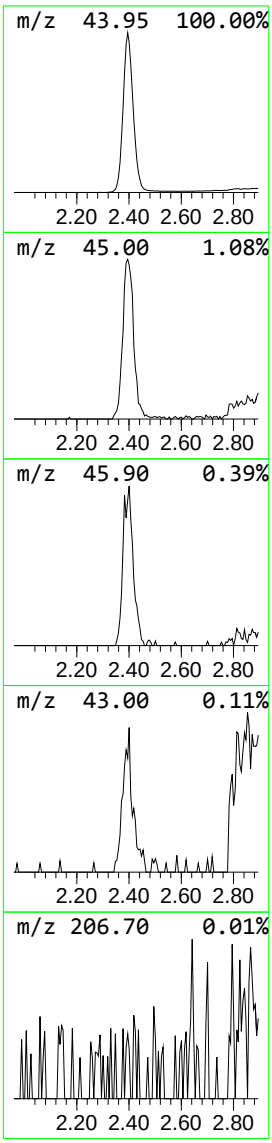
****

Peak Number 1 Carbon dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.395	276.18 ug/l	4977980	Pentafluorobenzene	8.483

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbon dioxide	44	CO2	000124-38-9	4
2	Nitrous oxide	44	N2O	010024-97-2	3
3	Acetaldehyde	44	C2H4O	000075-07-0	2
4	Acetonitrile-d3	44	C2D3N	002206-26-0	2
5	Ethyne, fluoro-	44	C2HF	002713-09-9	2





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Data File : VN081084.D
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Operator : JC\MD
Sample : P1528-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
IDW-20240215

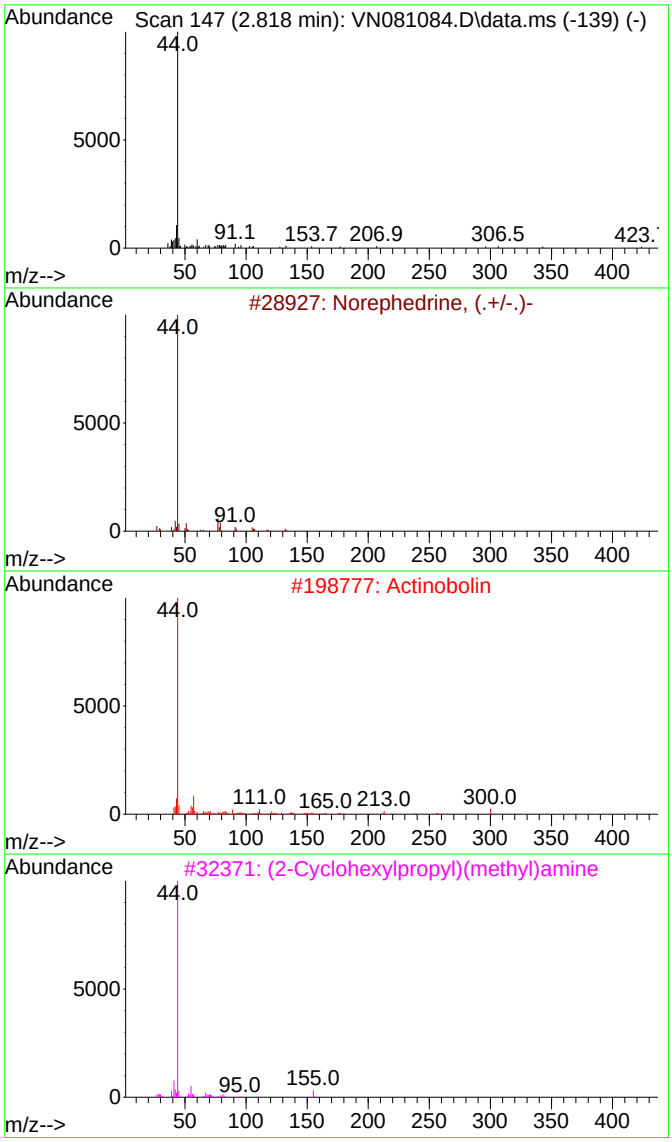
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

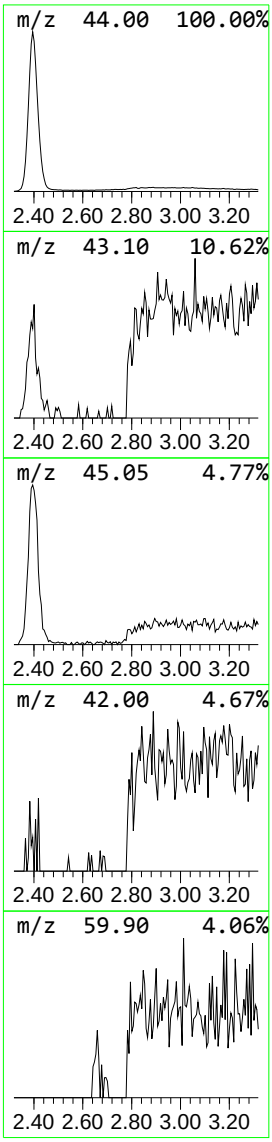
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Norephedrine, (.+/-.)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.818	5.09 ug/l	91783	Pentafluorobenzene	8.483

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Norephedrine, (.+/-.)-	151	C9H13NO	014838-15-4	38
2	Actinobolin	300	C13H20N2O6	024397-89-5	38
3	(2-Cyclohexylpropyl)(methyl)amine	155	C10H21N	000532-52-5	38
4	n-Hexylmethylamine	115	C7H17N	035161-70-7	38
5	1,2-Propanediamine	74	C3H10N2	000078-90-0	9





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Operator : JC\MD
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Instrument :
MSVOA_N
ClientSampleId :
IDW-20240215

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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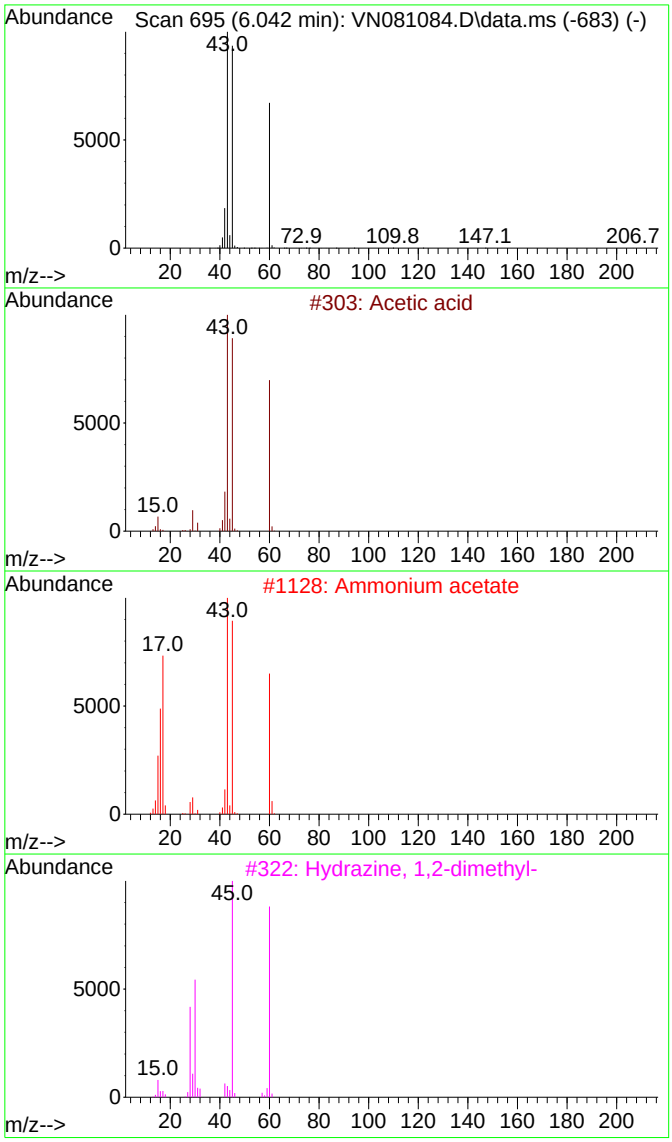
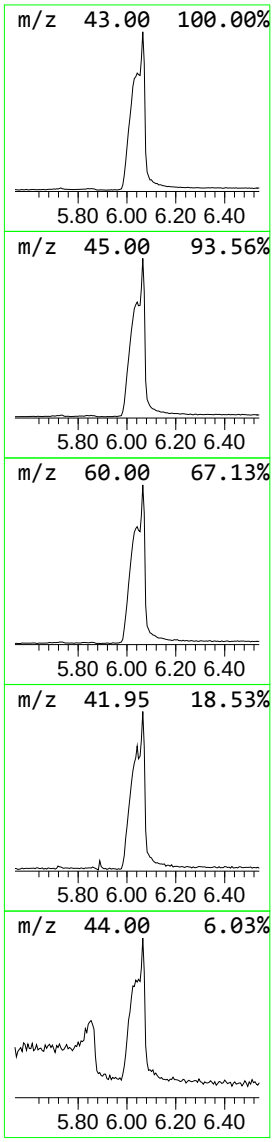
Peak Number 3 Acetic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.042	346.24 ug/l	6240850	Pentafluorobenzene	8.483

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	90
2	Ammonium acetate	77	C2H7NO2	000631-61-8	74
3	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	64
4	Carbonyl sulfide	60	COS	000463-58-1	5
5	Thiirane	60	C2H4S	000420-12-2	5





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ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
IDW-20240215

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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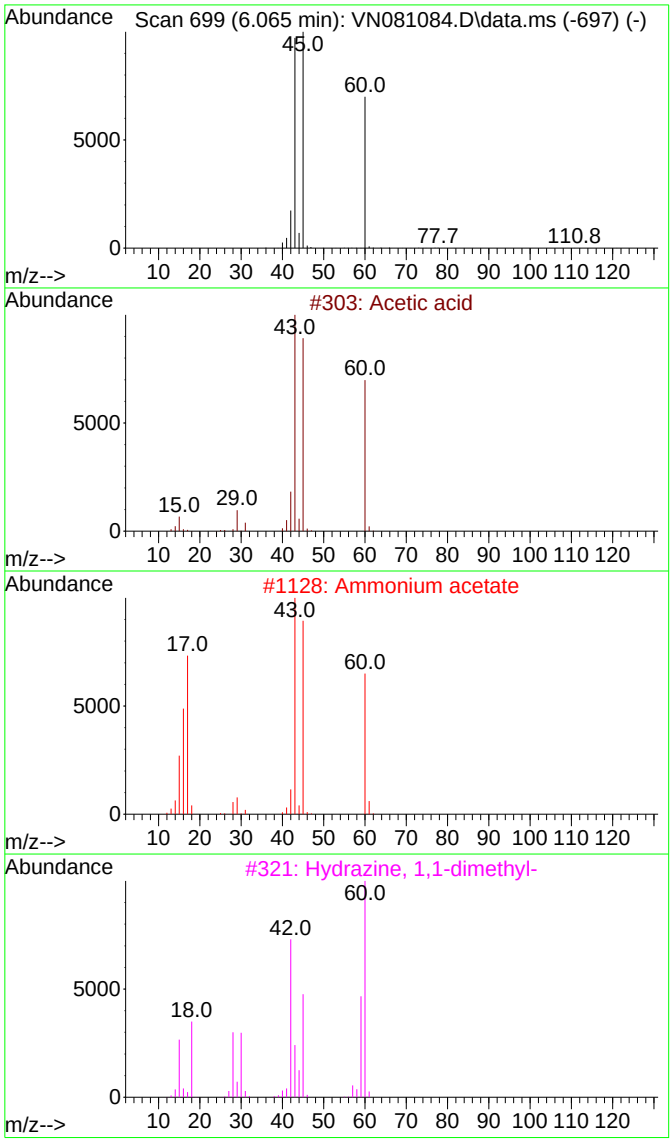
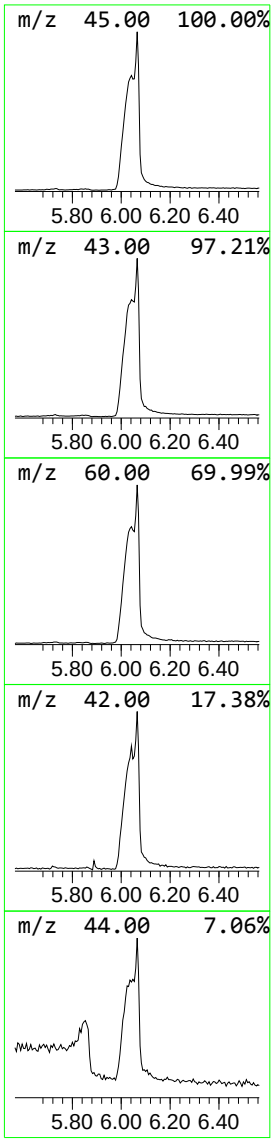
Peak Number 4 Acetic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.065	185.34 ug/l	3340630	Pentafluorobenzene	8.483

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	90
2	Ammonium acetate	77	C2H7NO2	000631-61-8	74
3	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
4	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	5
5	Hydrogen isocyanate	43	CHNO	000075-13-8	5





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021924\
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Acq On : 19 Feb 2024 18:29
Operator : JC\MD
Sample : P1528-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
IDW-20240215

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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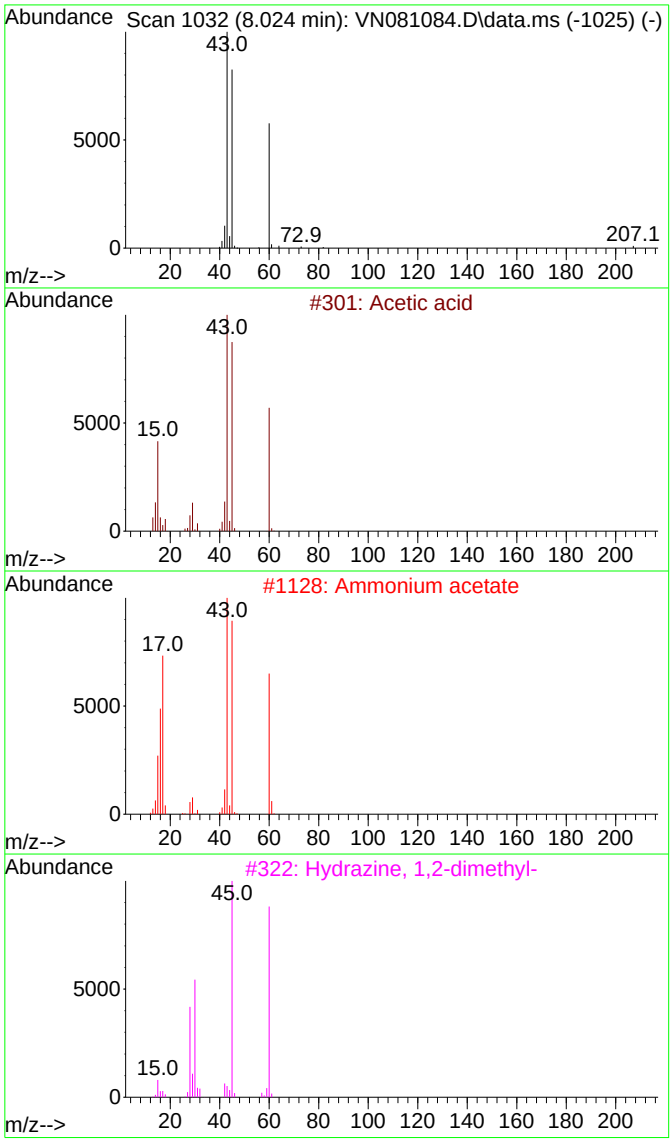
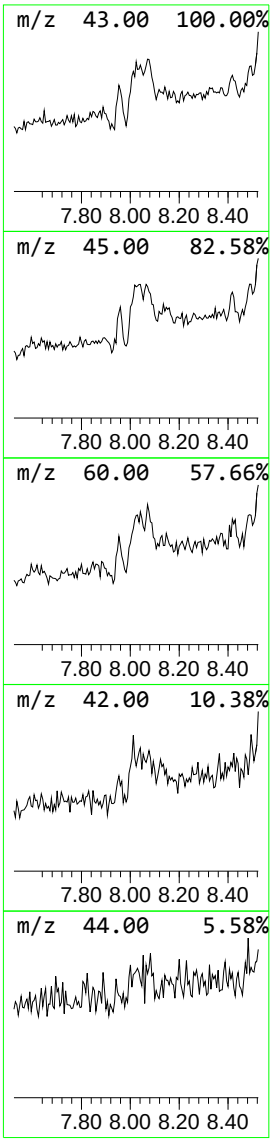
Peak Number 5 Acetic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.024	9.13 ug/l	164506	Pentafluorobenzene	8.483

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	90
2	Ammonium acetate	77	C2H7NO2	000631-61-8	74
3	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	50
4	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
5	Butanoic acid, 3-hydroxy-	104	C4H8O3	000300-85-6	9





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Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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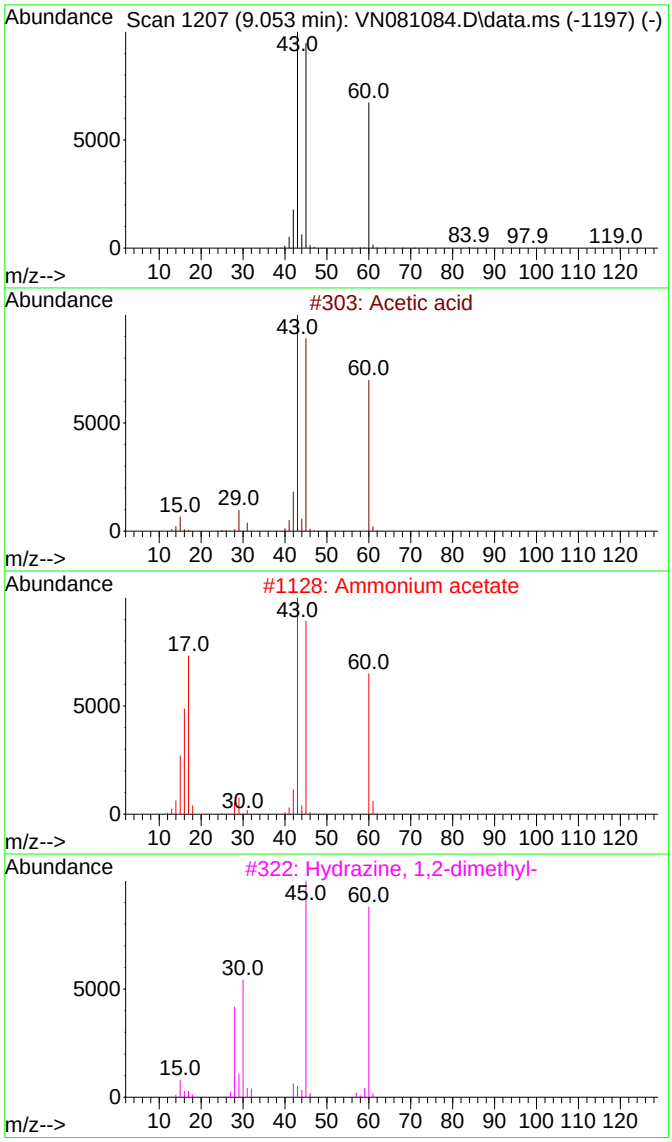
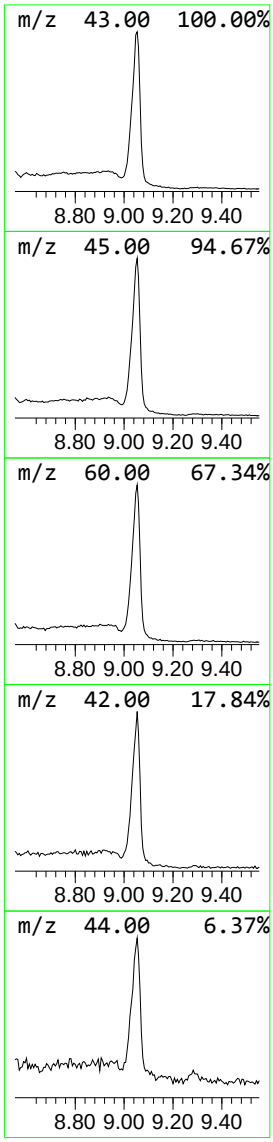
Peak Number 6 Acetic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.053	141.12 ug/l	4267770	1,4-Difluorobenzene	9.288

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	91
2	Ammonium acetate	77	C2H7NO2	000631-61-8	74
3	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	64
4	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
5	Thiirane	60	C2H4S	000420-12-2	5





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Instrument :
MSVOA_N
ClientSampleId :
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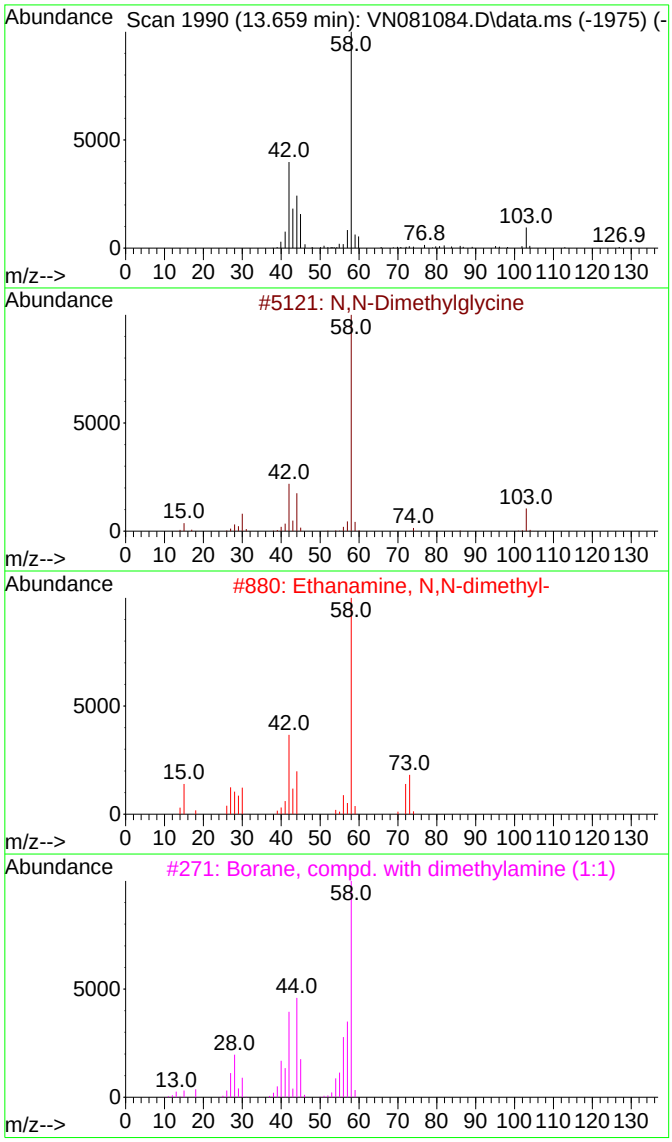
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

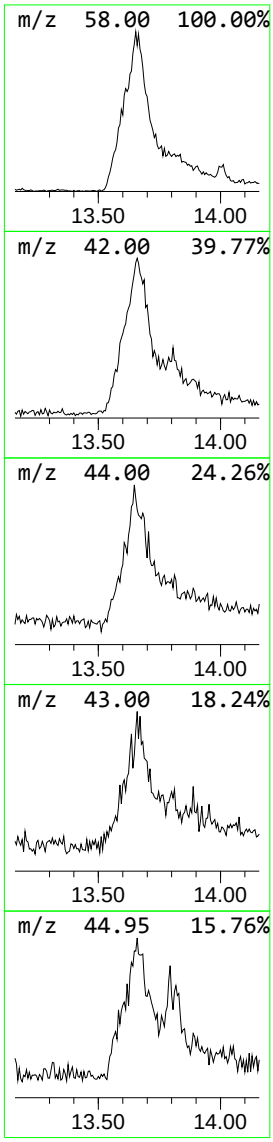
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 N,N-Dimethylglycine Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.659	24.32 ug/l	775914	1,4-Dichlorobenzene-d4	13.806

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N,N-Dimethylglycine	103	C4H9NO2	001118-68-9	53
2	Ethanamine, N,N-dimethyl-	73	C4H11N	000598-56-1	50
3	Borane, compd. with dimethylamin...	59	C2H10BN	000074-94-2	45
4	1-Propanone, 1-(1-adamantyl)-3-d...	235	C15H25NO	031878-58-7	40
5	Carbamic acid, 2-(dimethylamino)...	132	C5H12N2O2	004220-32-0	40





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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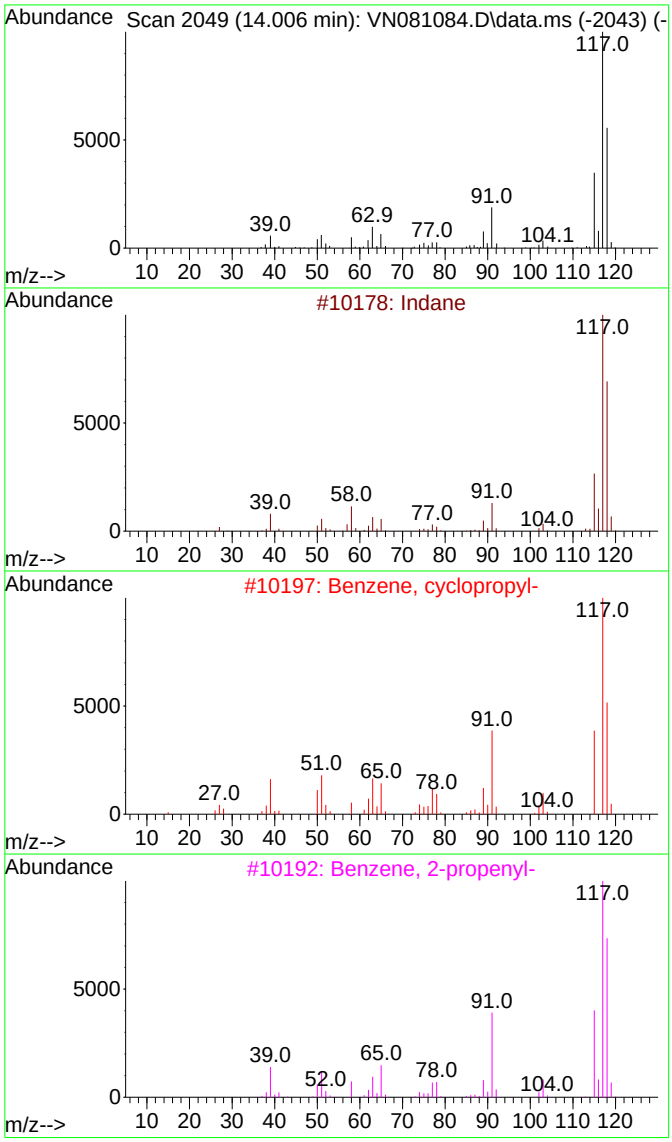
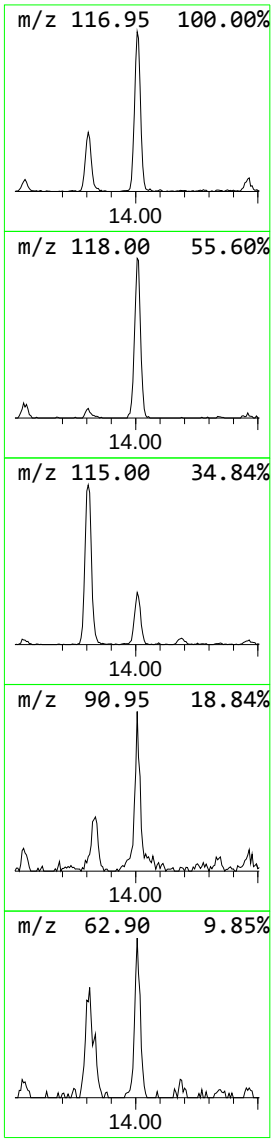
Peak Number 8 Indane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.006	12.81 ug/l	408629	1,4-Dichlorobenzene-d4	13.806

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	72
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	59
4	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	49
5	Indole	117	C8H7N	000120-72-9	47





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Instrument :
MSVOA_N
ClientSampleId :
IDW-20240215

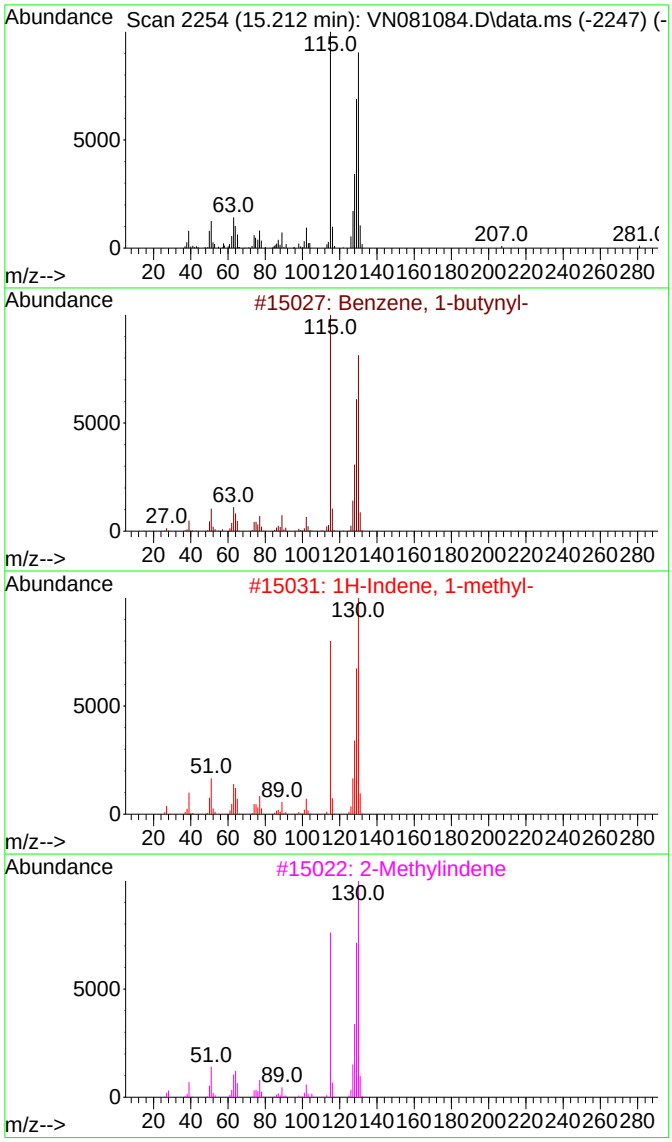
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

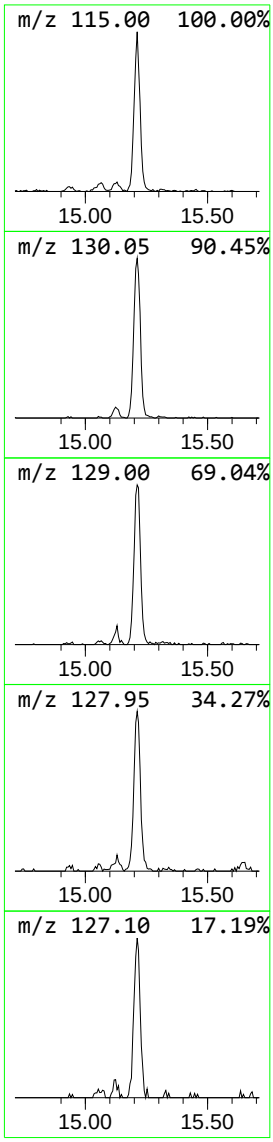
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-butynyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.212	13.63 ug/l	434968	1,4-Dichlorobenzene-d4	13.806

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-butynyl-	130	C10H10	000622-76-4	96
2	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	95
3	2-Methylindene	130	C10H10	002177-47-1	95
4	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	95
5	1,4-Dihydronaphthalene	130	C10H10	000612-17-9	93





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard		
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Carbon dioxide	2.395	276.2	ug/l	4977980	1	8.483	901222	50.0
Norephedrine, (...	2.818	5.1	ug/l	91783	1	8.483	901222	50.0
Acetic acid	6.042	346.2	ug/l	6240850	1	8.483	901222	50.0
Acetic acid	6.065	185.3	ug/l	3340630	1	8.483	901222	50.0
Acetic acid	8.024	9.1	ug/l	164506	1	8.483	901222	50.0
Acetic acid	9.053	141.1	ug/l	4267770	2	9.288	1512130	50.0
N,N-Dimethylgly...	13.659	24.3	ug/l	775914	4	13.806	1595190	50.0
Indane	14.006	12.8	ug/l	408629	4	13.806	1595190	50.0
Benzene, 1-buty...	15.212	13.6	ug/l	434968	4	13.806	1595190	50.0